

## **Phase Diagrams of Bend Spherocylinders**

J. Orozco and J. Mulia

*Facultad de Ciencias*

*UAEMEX*

*Instituto Literario 100*

*Col. Centro*

*C.P. 50000, Toluca, México*

Using both NVT and NPT Monte Carlo simulation we compute phase diagrams of "elbows" (bend spherocylinders). Actually the elbows are made of two equal spherocylinders joined by their ends at certain fixed angle. In order to generate the new orientation we make the following steps. First, we draw a line between the center of mass of each spherocylinder. This line is change randomly about the middle point of the centers of mass as usual. Finally, we rotate the complete elbow around this line to obtain the new orientation of the elbow. The new position of the center of mass is obtained in the usual way. Then we follow with the usual acceptance criteria. In the first calculations we found that no liquid crystal phase is possible if the total length to diameter ratio is less than 5, if the angle between both spherocylinders is no greater than 25 degrees. However if the ratio is bigger than 5 the same old phases are found. But if the angle between the spherocylinders is bigger once again no liquid crystal phase is present. By now we are performing calculations for elbows with unequal spherocylinders. The rotations are performed in a similar way as before. We think a new phase is present in this case, but more calculations have to be made.